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Computation of Jacobi functions of the second kind for use in nearside–farside scattering theory

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Abstract

The nearside–farside decomposition of a partial wave series is currently being used to understand the angular scattering of atom–diatom collision systems. In this theory, it is necessary to compute Jacobi functions of the second kind on the cut. These functions are denoted by $Q_n^{(\alpha,\beta)}(\cos\theta)$, where n, α, β, may be large positive integers. The $Q_n^{(\alpha,\beta)}(\cos\theta)$ can be computed from a three-term linear recurrence relation provided the initial values corresponding to $n = 0$ and 1, are known. We derive explicit formulas for $Q_0^{(\alpha,\beta)}(\cos\theta)$, $Q_1^{(\alpha,\beta)}(\cos\theta)$ in terms of elementary transcendental functions. A new generating function for Jacobi functions of nonintegral degree off the cut is obtained, a special case of which yields a generating function for $Q_n^{(\alpha,\beta)}(\cos\theta)$. This is used to check the numerical results, as is a Casoratian relation. We show that the recurrence for $Q_n^{(\alpha,\beta)}(\cos\theta)$ is stable in the forward direction with errors growing like $O(n)$. We also present some numerics demonstrating the success of the method.

Keywords: Error propagation; Difference equations; Recurrence relations; Jacobi functions of the first kind; Jacobi functions of the second kind; Jacobi polynomials; generating functions; Nearside–farside theory; Appell hypergeometric functions; Partial wave series; Scattering amplitude; Angular scattering; Atom–atom collisions; Atom–diatom collisions

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1. Introduction

Nearside–farside scattering theory has often been used to understand nuclear heavy-ion differential cross sections [13]. Recently, the first application of nearside–farside ideas to atom–atom and atom–diatom collisions has been reported, [4, 14–16, 12].

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The starting point for a nearside–farside analysis is the partial-wave series representation of the scattering amplitude. Mathematically, a partial-wave series is an infinite series in a basis set of appropriate special functions; the coefficients in the series contain information on the scattering dynamics. The special functions can be Legendre polynomials, associated Legendre functions, or reduced rotation matrix elements, which are related to Jacobi polynomials. The next step is a nearside–farside decomposition of the basis functions into travelling angular waves; these correspond to scattering from the nearside and farside of the target.

As an example, consider the scattering amplitude for an elastic, inelastic or reactive A + BC molecular collision. The partial-wave series representation of the scattering amplitude is

$$f_{m_f, m_i}(\theta) = \sum_{J=0}^{\infty} a_J^{(m_f, m_i)} d^J_{m_f, m_i}(\theta), \tag{1.1}$$

see [12], where θ is the scattering angle, J is the total angular momentum quantum number, m_f, m_i are helicity quantum numbers for the final and initial states, respectively, and $d^J_{m_f, m_i}(\theta)$ is a reduced rotation matrix element as defined in [6]. Possible values for m_f, m_i are 0, ± 1, $\pm 2, \ldots, \pm J$. However, by means of symmetry relations obeyed by the reduced rotation matrix elements it is possible to use values for m_f, m_i such that $m_f + m_i$ and $m_f - m_i$ are always positive integers or zero, [12]. In what follows, we shall assume this has been done.

The reduced rotation matrix element is related to the Jacobi polynomial $P_n^{(\alpha,\beta)}(\cos\theta)$ by

$$\begin{aligned} d^J_{m_f, m_i}(\theta) &= N^J_{m_f, m_i}[\sin(\theta/2)]^{m_f - m_i}[\cos(\theta/2)]^{m_f + m_i} \\ &\quad \times P^{(\alpha,\beta)}_{J-m_f}(\cos\theta), \quad \alpha = m_f - m_i, \quad \beta = m_f + m_i, \end{aligned} \tag{1.2}$$

where $N^J_{m_f, m_i}$ is a normalization factor [12].

The next step is the decomposition of $P_n^{(\alpha,\beta)}(\cos\theta)$ into nearside and farside components, $H_n^{(\alpha,\beta)-}(\cos\theta)$ and $H_n^{(\alpha,\beta)+}(\cos\theta)$, respectively,

$$P_n^{(\alpha,\beta)}(\cos\theta) = H_n^{(\alpha,\beta)+}(\cos\theta) + H_n^{(\alpha,\beta)-}(\cos\theta), \tag{1.3}$$

subject to the asymptotic constraint

$$H_n^{(\alpha,\beta)\pm}(\cos\theta) \sim \tfrac{1}{2}(\pi n)^{-1/2} g_{\alpha,\beta}(\theta)\exp\{\pm i[N_{\alpha,\beta}\theta - \tfrac{1}{2}\pi\alpha - \tfrac{1}{4}\pi]\}, \quad n \to \infty, \tag{1.4}$$

where

$$g_{\alpha,\beta}(\theta) = [\sin(\theta/2)]^{-\alpha-1/2}[\cos(\theta/2)]^{-\beta-1/2},$$

and

$$N_{\alpha,\beta} = n + \tfrac{1}{2}(\alpha + \beta + 1).$$

Such a decomposition is possible because the Jacobi polynomial behaves asymptotically like a pure cosine, see Section 5.

The explicit representation of the nearside–farside decomposition in [12] is

$$H_n^{(\alpha,\beta)\pm}(\cos\theta) = \frac{1}{2}\left[P_n^{(\alpha,\beta)}(\cos\theta) \mp \left(\frac{2i}{\pi}\right) e^{i\pi\alpha} Q_n^{(\alpha,\beta)}(\cos\theta)\right],$$

where $Q_n^{(\alpha,\beta)}(\cos\theta)$ is the Jacobi function of the second kind as defined by [18, p.78, (4.62.9)] or [8, v 2, p.171, (22)]. An alternative definition of the Jacobi function due to [5] can also be used—see [12] for details.

Thus, to compute the nearside and farside components, we must evaluate two series: a series of Jacobi polynomials and a series of Jacobi functions. A computation involves calculating each function for a large range of indices $n = 0, 1, 2, \ldots, N$ with $N = 200$ for typical applications in atom–diatom scattering.

The series of Jacobi polynomials poses no special problem. The required sequence of polynomials may be computed stably for fixed θ using the linear recurrence relation for the polynomials, either in the backward or in the forward direction, see [20]. For the forward computation, the required initial values $P_0^{(\alpha,\beta)}(\cos\theta)$ and $P_1^{(\alpha,\beta)}(\cos\theta)$ are trivial: a constant and a linear function, respectively. Furthermore, there are a number of known expansions, namely, generating functions, which can be used as checks on the computation.

The series of Jacobi functions is a much more difficult problem. Although the recurrence relation for these functions is the same as that satisfied by the polynomials and is stable in either direction, the initial values $Q_0^{(\alpha,\beta)}(\cos\theta)$ and $Q_1^{(\alpha,\beta)}(\cos\theta)$ are, for general α and β, higher transendental functions. A major analytical and computational effort is required just to start the calculations. Also, there seems to be no normalization relationships for these functions, e.g., generating functions, which can be used to check the computations.

The purpose of this paper is to show how both these problems can be overcome. Section 2 establishes our notation and reports the basic formulas we shall use. Section 3 shows that for α, β, integers, the Jacobi functions can be written in terms of elementary algebraic and logarithmic functions (a fact that does not seem to be generally known), although these functions become rather complicated for large α, β. In particular, we obtain explicit formulas for $Q_0^{(\alpha,\beta)}(\cos\theta)$ and $Q_1^{(\alpha,\beta)}(\cos\theta)$. In Section 4, we deduce a new generating function for these functions, which we use as a computational check. This generating function is a special case of a more general one for Jacobi functions of nonintegral degree off the cut. The error propagation in the recurrence relation for the $Q_n^{(\alpha,\beta)}(\cos\theta)$ is examined in Section 5. Numerical results in the form of tables and graphs are reported in Section 6. Our conclusions are in Section 7.

We remark that the computation of Jacobi functions seems to be unexplored territory. The recent review by Lozier and Olver of the literature on the evaluation of the special functions, [10], contains no relevant material, so the present paper is, apparently, the first to give an algorithm for the evaluation of these functions.

2. Notation and basic formulas

Our notation will mostly follow that of the Bateman volumes [8]. We define the Jacobi polynomial of degree n by [8, vol. 2, p.170, (16)]:

$$P_n^{(\alpha,\beta)}(z) = \frac{\Gamma(n+\alpha+1)}{\Gamma(n+1)\Gamma(\alpha+1)}\, {}_2F_1\left(\begin{matrix} -n, n+\alpha+\beta+1 \\ \alpha+1 \end{matrix}; \frac{1-z}{2}\right),$$

$$\alpha > -1, \quad \beta > -1, \quad n = 0, 1, 2, \ldots. \tag{2.1}$$

where z is a complex variable, Γ is the gamma function and ${}_2F_1(\,)$ is the Gaussian hypergeometric function, [8, vol. 1, Ch. II].[1] We define the Jacobi function (sometimes called the Jacobi function of the second kind) by the formula [8, vol. 2, p.170, (18)]:

$$Q_n^{(\alpha,\beta)}(z) = \frac{2^{n+\alpha+\beta}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(2n+\alpha+\beta+2)(z-1)^{n+\alpha+1}(z+1)^{\beta}}\,{}_2F_1\left(\begin{matrix} n+1, n+\alpha+1 \\ 2n+\alpha+\beta+2 \end{matrix}; \frac{2}{1-z}\right),$$

$$\alpha > -1, \quad \beta > -1, \quad n = 0,1,2,\ldots, \quad z \notin [-1,1]. \tag{2.2}$$

The Jacobi function has $[-1,1]$ as a branch cut. For values of $z = x = \cos\theta$ interior to this cut, we define the function to be the average of its values above and below the cut,[2] [8, vol. 2, p.171, (22)]:

$$\mathcal{Q}_n^{(\alpha,\beta)}(x) = \tfrac{1}{2}[Q_n^{(\alpha,\beta)}(x+\mathrm{i}0) + Q_n^{(\alpha,\beta)}(x-\mathrm{i}0)], \quad n = 0,1,2,\ldots, \quad x \in (-1,1), \tag{2.3}$$

which is a real analytic function of x.

An explicit (but complicated) expression for this function is given in [8, vol. 2, p.171, (23)]:

$$\mathcal{Q}_n^{(\alpha,\beta)}(x) = -\frac{\pi}{2}\operatorname{cosec}(\pi\alpha)P_n^{\alpha,\beta}(x) + 2^{\alpha+\beta-1}\cos(\pi\alpha)\frac{\Gamma(\alpha)\Gamma(n+\beta+1)}{\Gamma(n+\alpha+\beta+1)(1-x)^{\alpha}(1+x)^{\beta}}$$

$$\times\,{}_2F_1\left(\begin{matrix} n+1, -n-\alpha-\beta \\ 1-\alpha \end{matrix}; \frac{1-x}{2}\right), \quad \alpha > -1, \quad \beta > -1, \quad n = 0,1,2,\ldots, \quad x \notin (-1,1). \tag{2.4}$$

Strictly speaking, the representation holds only if α is not an integer, although if α is an integer, a limit can be taken which makes the expression meaningful. Essentially, it is the same type of limiting process that is used to define the Bessel function of the second kind $Y_n(z)$ from the function $Y_v(z)$, see [8, vol. 2, p.7].

The following integral representation will prove useful in Sections 3 and 4:

$$Q_n^{(\alpha,\beta)}(z) = \frac{1}{2^{n+1}(z-1)^{\alpha}(z+1)^{\beta}}\int_{-1}^{1}\frac{(1-t)^{n+\alpha}(1+t)^{n+\beta}}{(z-t)^{n+1}}\,\mathrm{d}t, \quad z \notin [-1,1]. \tag{2.5}$$

See [8, vol. 2, p.172, (28)]. This representation holds for z complex and off the cut $[-1,1]$, α, β, n complex, provided $\mathrm{Re}(n+\alpha) > -1$, $\mathrm{Re}(n+\beta) > -1$. This feature allows us to use the integral in Section IV to derive a generating function valid for general values of the parameters.

$P_n^{(\alpha,\beta)}(z)$, $Q_n^{(\alpha,\beta)}(z)$, and hence $\mathcal{Q}_n^{(\alpha,\beta)}(x)$ all satisfy the three-term linear recurrence relation, [8, vol. 2, p.169, (11), p.170],

$$y_{n+2}(z) + A_n(z)y_{n+1}(z) + B_n y_n(z) = 0, \quad n = 0,1,2,\ldots,$$

[1] Later, we will take n in this definition to be nonintegral. Then it will be necessary to require $|\arg(1+z)| < \pi$.

[2] We adopt the convention $(z-1)^{\alpha} = |z-1|^{\alpha}\mathrm{e}^{\mathrm{i}\alpha\phi}$, α real, with $\phi = 0$ for z real and >1. This implies $\arg(z-1) = \pm\pi$ for $z = \cos\theta \pm \mathrm{i}0$. See also [9, p.51].

where

$$A_n(z) = \frac{-(2n+\alpha+\beta+3)[(2n+\alpha+\beta+2)(2n+\alpha+\beta+4)z+\alpha^2-\beta^2]}{2(n+2)(n+\alpha+\beta+2)(2n+\alpha+\beta+2)},$$

$$B_n = \frac{(n+\alpha+1)(n+\beta+1)(2n+\alpha+\beta+4)}{(n+2)(n+\alpha+\beta+2)(2n+\alpha+\beta+2)}. \tag{2.6}$$

All the above functions can be computed from this recurrence if the initial values for $n = 0$ and 1 are known. For the polynomials, this presents no problem. However, the Jacobi functions are transcendental functions, and the computation of their initial values is nontrivial.

Evaluation of the Casoratian determinant of the recurrence gives a Wronskian-type relation for $P_n^{(\alpha,\beta)}(z)$ and $Q_n^{(\alpha,\beta)}(z)$,

$$P_n^{(\alpha,\beta)}(z)Q_{n-1}^{(\alpha,\beta)}(z) - P_{n-1}^{(\alpha,\beta)}(z)Q_n^{(\alpha,\beta)}(z)$$
$$= \frac{2^{\alpha+\beta-1}(2n+\alpha+\beta)\Gamma(n+\alpha)\Gamma(n+\beta)}{n!\,\Gamma(n+\alpha+\beta+1)(z-1)^{\alpha}(z+1)^{\beta}}, \quad n = 1,2,\ldots, \quad z \notin [-1,1]. \tag{2.7}$$

See [8, vol. 2, p.172, (26)]. On the cut we have

$$P_n^{(\alpha,\beta)}(x)Q_{n-1}^{(\alpha,\beta)}(x) - P_{n-1}^{(\alpha,\beta)}(x)Q_n^{(\alpha,\beta)}(x)$$
$$= \cos(\pi\alpha)\frac{2^{\alpha+\beta-1}(2n+\alpha+\beta)\Gamma(n+\alpha)\Gamma(n+\beta)}{n!\,\Gamma(n+\alpha+\beta+1)(1-x)^{\alpha}(1+x)^{\beta}}, \quad n = 1,2,\ldots. \tag{2.8}$$

The validity of (2.6)–(2.8) can be extended to α, β complex provided $\mathrm{Re}(n+\alpha) > -1$, $\mathrm{Re}(n+\beta) > -1$, although our values of α and β and n will be nonnegative integral.

The right-hand side of the identity (2.8) vanishes for $\alpha = \frac{1}{2}$ odd integer, which implies that $P_n^{(\alpha,\beta)}(x)$ and $Q_n^{(\alpha,\beta)}(x)$ are then no longer linearly independent. Eq. (2.4) shows that we have $Q_n^{(\alpha,\beta)}(x) = (-1)^{\alpha+1/2}\frac{1}{2}\pi P_n^{(\alpha,\beta)}(x)$.

3. Computational algorithm and initialization

We shall compute the Jacobi function $Q_n^{(\alpha,\beta)}(x)$ by utilizing the recurrence relation (2.6) in the forward direction starting with the initial values $y_0(x) = Q_0^{(\alpha,\beta)}(x)$, $y_1(x) = Q_1^{(\alpha,\beta)}(x)$. We are interested in $x = \cos\theta$ values interior to the cut, $-1 < x < 1$, i.e., $0 < \theta < \pi$.

In general, the Jacobi function is a higher transcendental function. We shall show that when α, β are nonnegative integers (as we will assume is the case from now on in this section), the functions reduce to elementary transcendental functions. We start with the relationship (2.5). We can write

$$(1-t)^{n+\alpha}(1+t)^{n+\beta} = \sum_{k=0}^{2n+\alpha+\beta} \frac{\mu_{n,k}^{(\alpha,\beta)}(z)(t-z)^k}{k!},$$

$$\mu_{n,k}^{(\alpha,\beta)}(z) = \frac{\mathrm{d}^k}{\mathrm{d}z^k}\{(1-z)^{n+\alpha}(1+z)^{n+\beta}\}, \quad \alpha, \beta = 0, 1, 2, \ldots . \tag{3.1}$$

Note that $\mu_{n,k}^{(\alpha,\beta)}(z)$ is a polynomial in z of degree $2n+\alpha+\beta-k$. It can be expressed in terms of $P_k^{(\alpha+n-k,\beta+n-k)}(z)$, see [8, vol. 2, p.169, (10)], so $\mu_{n,k}^{(\alpha,\beta)}(z)$ itself may be computed by means of a recurrence relation. In practice, we found it more convenient to use a computer algebra software package or Leibnitz's theorem. Putting (3.1) into (2.5) gives

$$Q_n^{(\alpha,\beta)}(z) = \frac{(z-1)^{-\alpha}(z+1)^{-\beta}}{2^{n+1}} \left\{ \sum_{\substack{k=0 \\ k \neq n}}^{2n+\alpha+\beta} \frac{\mu_{n,k}^{(\alpha,\beta)}(z)(-1)^k[(z+1)^{k-n} - (z-1)^{k-n}]}{k!(k-n)} + \frac{(-1)^n \mu_{n,n}^{(\alpha,\beta)}(z)}{n!} \ln\left(\frac{z+1}{z-1}\right) \right\}, \quad z \notin [-1, 1]. \tag{3.2}$$

On the cut we have

$$Q_n^{(\alpha,\beta)}(x) = \frac{(x-1)^{-\alpha}(x+1)^{-\beta}}{2^{n+1}} \left\{ \sum_{\substack{k=0 \\ k \neq n}}^{2n+\alpha+\beta} \frac{\mu_{n,k}^{(\alpha,\beta)}(x)(-1)^k[(x+1)^{k-n} - (x-1)^{k-n}]}{k!(k-n)} + \frac{(-1)^n \mu_{n,n}^{(\alpha,\beta)}(x)}{n!} \ln\left(\frac{1+x}{1-x}\right) \right\}. \tag{3.3}$$

(Remember, α, β, are integers.) In particular, for $n = 0$, we have

$$Q_0^{(\alpha,\beta)}(x) = \frac{(x-1)^{-\alpha}(x+1)^{-\beta}}{2} \sum_{k=1}^{\alpha+\beta} \frac{L_k^{(\alpha,\beta)}(x)(-1)^k[(x+1)^k - (x-1)^k]}{kk!} + (-1)^\alpha \tfrac{1}{2} \ln\left(\frac{1+x}{1-x}\right), \quad L_k^{(\alpha,\beta)}(x) = \mu_{0,k}^{(\alpha,\beta)}(x) = \frac{\mathrm{d}^k}{\mathrm{d}x^k}\{(1-x)^\alpha(1+x)^\beta\}. \tag{3.4}$$

(Empty sums are interpreted as 0.) $Q_1^{(\alpha,\beta)}(x)$ can also conveniently be obtained in terms of $Q_0^{(\alpha,\beta)}(x)$ from the formula (2.8). We find that

$$Q_1^{(\alpha,\beta)}(x) = \frac{-(x-1)^{-\alpha}(x+1)^{-\beta}2^{\alpha+\beta-1}(\alpha+\beta+2)\alpha!\beta!}{(\alpha+\beta+1)!} + \left[\frac{\alpha-\beta+(\alpha+\beta+2)x}{2}\right] Q_0^{(\alpha,\beta)}(x). \tag{3.5}$$

We thus have obtained explicit expressions for the initial values $y_0(x)$, $y_1(x)$ required in the recurrence relation (2.6).

4. Normalization relationships

As an aid in computing special functions from recurrence relations, normalization relationships are very useful. They may serve as a check on the computations or, if initial values are not available, as an intrinsic part of the computational format. The normalization relationship may be a generating function, say,

$$f(z) = \sum_{n=0}^{\infty} a_n y_n(z), \tag{4.1}$$

where $y_n(z)$ is the sequence to be computed, or some other type of formula relating the members of the desired sequence to one another. A useful relationship involving the Jacobi functions $Q_n^{(\alpha,\beta)}(x)$ is the Casoratian determinant (2.8), which also requires the values $P_n^{(\alpha,\beta)}(x)$ and $P_{n-1}^{(\alpha,\beta)}(x)$. It is no problem to generate the sequence $P_n^{(\alpha,\beta)}(x)$ from the recurrence along with the Jacobi functions, especially since the required initial values for the polynomials are simple, [18, p.71],

$$P_0^{(\alpha,\beta)}(x) = 1, \qquad P_1^{(\alpha,\beta)}(x) = \tfrac{1}{2}[(\alpha + \beta + 2)x + (\alpha - \beta)]. \tag{4.2}$$

We have found that formula (2.8) provides an excellent check, see Table 1, where $n = 200$ and the discussion in Section 6.

Numerous generating functions are known for the $P_n^{(\alpha,\beta)}(z)$ or, more generally for the $P_{n+c}^{(\alpha,\beta)}(z)$, where $c \geqslant 0$. (Actually, c can be complex.) Such functions are sometimes called Jacobi functions (of the first kind.) The definition is just that of the polynomials $P_n^{(\alpha,\beta)}(z)$, (2.1), except n may be nonintegral. The Jacobi functions of the first kind can be analytically continued in the z-plane cut along $(-\infty, -1]$. (We will obtain a little added generality in this section by considering the argument of all Jacobi functions to be complex.) One such generating function is[3]

$$\sum_{n=0}^{\infty} \frac{(\alpha + \beta + c + 1)_n (c + 1)_n}{n!(e)_n} \lambda^n P_{n+c}^{(\alpha,\beta)}(z) = \frac{\Gamma(\alpha + c + 1)}{\Gamma(\alpha + 1)\Gamma(c + 1)}$$
$$\times \left(\frac{1 + z}{2}\right)^{-c-\alpha-\beta-1} F_4\left(\alpha + c + 1, \alpha + \beta + c + 1; \alpha + 1, e; \frac{z - 1}{z + 1}, \frac{2\lambda}{z + 1}\right). \tag{4.3}$$

This expansion may be obtained by identifying the Gaussian hypergeometric function in the expansion [21, (22)],

$$\sum_{n=0}^{\infty} \frac{(a + c)_n (b)_n t^n}{n!(e)_n} {}_2F_1\left(\begin{matrix} -n - a, \ n + b \\ c \end{matrix}; x\right)$$
$$= (1 - x)^{-b} F_4\left(a + c, b; c, e; \frac{-x}{1 - x}, \frac{t}{1 - x}\right), \tag{4.4}$$

[3] We shall not, in general, give the complicated conditions on the parameters α, β, e, etc. for which our expansions are valid. The terms in all of our expansions are analytic in these parameters and the reader can assume that the expansions, when they converge, are valid whenever both sides are analytic.

Table 1
The Casoratian identity (2.8) for $n = 200$, $\alpha = \beta = 6$. $P_n^{(\alpha,\beta)}(\cos\theta)$, $Q_n^{(\alpha,\beta)}(\cos\theta)$ are computed from the recurrence relation (2.6) for $n = 0, 1, 2, \ldots, 200$

$\theta/°$	Numerical values of left and right-hand sides of (2.8)	Relative error	Absolute error
1	0.2091732010734(+23)	−0.155(−31)	−0.324(−09)
2	0.5116110276117(+19)	−0.148(−31)	−0.755(−13)
3	0.3955194996092(+17)	0.398(−31)	0.158(−14)
4	0.1258217270125(+16)	0.148(−31)	0.186(−16)
5	0.8693962523568(+14)	0.795(−32)	0.691(−18)
6	0.9816463952851(+13)	−0.117(−31)	−0.115(−18)
7	0.1556095361836(+13)	0.109(−31)	0.169(−19)
8	0.3163051155497(+12)	−0.519(−32)	−0.164(−20)
9	0.7776435379480(+11)	0.143(−31)	0.111(−20)
10	0.2221913274516(+11)	0.715(−32)	0.159(−21)
20	0.6518529690617(+07)	0.520(−32)	0.339(−25)
30	0.6841161007370(+05)	0.609(−32)	0.417(−27)
40	0.3357066178850(+04)	0.317(−32)	0.106(−28)
50	0.4089990178322(+03)	0.518(−32)	0.212(−29)
60	0.9384308652085(+02)	0.460(−32)	0.431(−30)
70	0.3523222464564(+02)	0.490(−32)	0.173(−30)
80	0.2007023030840(+02)	0.461(−32)	0.924(−31)
90	0.1670205324065(+02)	0.369(−32)	0.616(−31)
100	0.2007023030840(+02)	0.445(−32)	0.894(−31)
110	0.3523222464564(+02)	0.542(−32)	0.191(−30)
120	0.9384308652085(+02)	0.460(−32)	0.431(−30)
130	0.4089990178322(+03)	0.458(−32)	0.187(−29)
140	0.3357066178850(+04)	0.435(−32)	0.146(−28)
150	0.6841161007370(+05)	0.517(−32)	0.353(−27)
160	0.6518529690617(+07)	0.359(−32)	0.234(−25)
170	0.2221913274516(+11)	−0.581(−32)	−0.129(−21)
171	0.7776435379480(+11)	0.408(−32)	0.318(−21)
172	0.3163051155497(+12)	−0.770(−32)	−0.244(−20)
173	0.1556095361836(+13)	0.135(−33)	0.210(−21)
174	0.9816463952851(+13)	0.138(−32)	0.136(−19)
175	0.8693962523568(+14)	0.245(−31)	0.213(−17)
176	0.1258217270125(+16)	0.295(−31)	0.371(−16)
177	0.3955194996092(+17)	−0.526(−33)	−0.208(−16)
178	0.5116110276117(+19)	−0.509(−31)	−0.260(−12)
179	0.2091732010734(+23)	−0.186(−31)	−0.389(−09)

Note: The numbers in parentheses are the power of ten by which the entry must be multiplied.

with a Jacobi function via (2.1). Eq. (4.4) is valid in a neighborhood of the (x, t) origin in C^2. Here $(a)_n = \Gamma(a+n)/\Gamma(a)$ and $F_4(\,)$ is an Appell hypergeometric function of two variables, see [2, Ch. IX].

When $e = 2c + \alpha + \beta + 2$, the $F_4()$ becomes the product of two ${}_2F_1()$'s, see [2, p.81, (2)],

$$F_4(\alpha, \beta; \gamma, \alpha + \beta - \gamma + 1; z(1 - Z), Z(1 - z))$$
$$= {}_2F_1\left(\begin{matrix}\alpha, \beta \\ \gamma\end{matrix}; 1 - Z\right) {}_2F_1\left(\begin{matrix}\alpha, \beta \\ \alpha + \beta - \gamma + 1\end{matrix}; 1 - z\right). \tag{4.5}$$

The resulting ${}_2F_1()$'s may then be identified in terms of Jacobi functions using (2.1) and (2.2). A very tedious computation gives

$$\sum_{n=0}^{\infty} \frac{(\alpha + \beta + c + 1)_n (c + 1)_n}{n!(2c + \alpha + \beta + 2)_n} \lambda^n P_{n+c}^{(\alpha,\beta)}(z)$$
$$= \frac{2\lambda^{-c-\alpha-\beta-1} \Gamma(2c + \alpha + \beta + 2)}{\Gamma(\alpha + c + 1)\Gamma(\beta + c + 1)} Q_c^{(\alpha,\beta)}(\omega_1) P_c^{(\alpha,\beta)}(\omega_2), \tag{4.6}$$

where here, and in what follows, we define

$$\omega_1 = \frac{1 + R}{\lambda}, \qquad \omega_2 = \frac{1 - R}{\lambda}, \qquad R = (1 - 2z\lambda + \lambda^2)^{1/2}. \tag{4.7}$$

Expansions (4.3) and (4.6) converge[4] for $|\lambda| < |z - (z^2 - 1)^{1/2}|$. The specialization (4.6) has been derived independently by several authors, see the references given in [21, 17, p.453] (The formula given in [17] has a misprint. The argument of the $Q_m^{(\alpha,\beta)}$ function, in these authors' notation, should be $(1 + \rho)/t$.) Note that c may be nonintegral in (4.6); then $Q_c^{(\alpha,\beta)}()$ is defined by (2.2).

Another interesting specialization of (4.3) occurs when we put $e = \alpha + \beta + c + 1$. Using the formula [2, p.102, (20ii)],

$$F_4\left(\alpha, \beta; \gamma, \beta; \frac{-x}{(1 - x)(1 - y)}, \frac{-y}{(1 - x)(1 - y)}\right)$$
$$= (1 - x)^\alpha (1 - y)^\alpha F_1(\alpha; \gamma - \beta, 1 + \alpha - \gamma; \gamma; x, xy), \tag{4.8}$$

gives

$$\sum_{n=0}^{\infty} \frac{(c + 1)_n}{n!} \lambda^n P_{n+c}^{(\alpha,\beta)}(z) = \frac{\Gamma(\alpha + c + 1)}{\Gamma(\alpha + 1)\Gamma(c + 1)} \left(\frac{\omega_2 - 1}{z - 1}\right)^{\alpha + c + 1}$$
$$\times \left(\frac{1 + z}{2}\right)^{-\beta} F_1\left(\alpha + c + 1; -\beta - c, c + 1; \alpha + 1; \frac{1 - \omega_2}{2}, \frac{\lambda(1 - \omega_2)^2}{2(z - 1)}\right), \tag{4.9}$$

where $F_1()$ denotes an Appell hypergeometric function of two variables, [2], Ch. IX.

[4] To determine the principal values in (4.7), we write $(1 - 2z\lambda + \lambda^2)^{1/2} = (Z_1 - \lambda)^{1/2} \cdot (Z_2 - \lambda)^{1/2}$, where $Z_1 = z + (z^2 - 1)^{1/2}$, $Z_2 = z - (z^2 - 1)^{1/2}$ and all square roots have their principal values.

We now put $c = 0$, $e = \alpha + \beta + c + 1$ in (4.3) and use [2, p.102, (20iii)],

$$F_4\left(\alpha, \beta; \alpha, \beta; \frac{-x}{(1-x)(1-y)}, \frac{-y}{(1-x)(1-y)}\right)$$

$$= (1-xy)^{-1}(1-x)^{\beta}(1-y)^{\alpha}. \tag{4.10}$$

The result is the standard generating function for $P_n^{(\alpha,\beta)}(z)$:

$$\sum_{n=0}^{\infty} \lambda^n P_n^{(\alpha,\beta)}(z) = 2^{\alpha+\beta} R^{-1}(1-\lambda+R)^{-\alpha}(1+\lambda+R)^{-\beta}, \tag{4.11}$$

see [8, vol. 2, p.172, (29)]. Expansions (4.9) and (4.11) also converge for $|\lambda| < |z-(z^2-1)^{1/2}|$.

We have not been able to find the $Q_{n+c}^{(\alpha,\beta)}(z)$ analog of expansions (4.6) or (4.9) in the literature. Strangely enough, the analog of (4.6) is buried in an exercise in Bailey's book, [2, p.100, (14)], which we write as

$$\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{(\alpha)_{m+n}(\beta)_{m+n}(\gamma-\alpha)_m(\gamma-\beta)_m}{m!\,n!(\gamma)_m(\gamma)_{2m+n}}(wW)^m(w+W-wW)^n$$

$$= {}_2F_1\left(\begin{matrix}\alpha, \beta \\ \gamma\end{matrix}; w\right) {}_2F_1\left(\begin{matrix}\alpha, \beta \\ \gamma\end{matrix}; W\right). \tag{4.12}$$

(This result is originally due to Watson [19].) Making use of the elementary properties of the $(a)_n$ symbol, we find the inner sum above may be interpreted as a Jacobi function of the second kind. The left-hand side is

$$\sum_{m=0}^{\infty} \frac{(\alpha)_m(\beta)_m(\gamma-\alpha)_m(\gamma-\beta)_m(wW)^m}{m!(\gamma)_m(\gamma)_{2m}}\, {}_2F_1\left(\begin{matrix}m+\alpha, m+\beta \\ 2m+\gamma\end{matrix}; w+W-wW\right). \tag{4.13}$$

Now let $wW = -2\lambda/(1-z)$, $w + W - wW = 2/(1-z)$, then identify the ${}_2F_1$ above as a Jacobi function by using (2.2) with α, β, γ, m replaced, respectively, by $c+1$, $c+\alpha+1$, $2c+\alpha+\beta+2$, n. We get the pretty result

$$\sum_{n=0}^{\infty} \frac{(\alpha+\beta+c+1)_n(c+1)_n}{n!(2c+\alpha+\beta+2)_n}\lambda^n Q_{n+c}^{(\alpha,\beta)}(z)$$

$$= \frac{2\lambda^{-c-\alpha-\beta-1}\Gamma(2c+\alpha+\beta+2)}{\Gamma(\alpha+c+1)\Gamma(\beta+c+1)} Q_c^{(\alpha,\beta)}(\omega_1) Q_c^{(\alpha,\beta)}(\omega_2). \tag{4.14}$$

The analog of (4.9) is obtained by replacing n by $n+c$ in (2.5), multiplying by $\lambda^n(c+1)_n/n!$ and summing under the integral sign. Using the following result, [2, p.77, (4)],

$$\frac{\Gamma(\alpha)\Gamma(\gamma-\alpha)}{\Gamma(\gamma)}F_1(\alpha;\beta,\beta';\gamma;x,y)$$
$$=\int_0^1 u^{\alpha-1}(1-u)^{\gamma-\alpha-1}(1-ux)^{-\beta}(1-uy)^{-\beta'}\,du, \tag{4.15}$$

we find

$$\sum_{n=0}^{\infty}\frac{(c+1)_n}{n!}\lambda^n Q_{n+c}^{(\alpha,\beta)}(z)=\frac{\Gamma(\alpha+c+1)\Gamma(\beta+c+1)2^{\alpha+\beta+c}}{\Gamma(2c+\alpha+\beta+2)}(z+1)^{-\beta-c-1}$$
$$\times(z-1)^{-\alpha}F_1\left(\beta+c+1;c+1;c+1;2c+\alpha+\beta+2;\frac{\lambda(1+\omega_2)}{z+1},\frac{\lambda(1+\omega_1)}{z+1}\right). \tag{4.16}$$

Expansions (4.14) and (4.16) converge for $|\lambda|<|z+(z^2-1)^{1/2}|$. Note that since $|z+(z^2-1)^{1/2}|>1>|z-(z^2-1)^{1/2}|=1/|z+(z^2-1)^{1/2}|$ for all z off the cut $[-1,1]$, the rate of convergence of (4.14) and (4.16) is exponentially faster than that of the expansions involving the $P_{n+c}^{(\alpha,\beta)}(\,)$ functions.

When $c=0$, (4.16) simplifies considerably. The portion containing ω_1 and ω_2 in the integrand in the integral representation for the $F_1(\,)$ function, see (4.15), can be decomposed by partial fractions. The result is the $Q_n^{(\alpha,\beta)}(z)$ analog of the classical generating function for the Jacobi polynomials:

$$\sum_{n=0}^{\infty}\lambda^n Q_n^{(\alpha,\beta)}(z)=\frac{1}{(\lambda^2-2z\lambda+1)^{1/2}}$$
$$\times\left\{\left(\frac{\omega_2-1}{z-1}\right)^{\alpha}\left(\frac{\omega_2+1}{z+1}\right)^{\beta}Q_0^{(\alpha,\beta)}(\omega_2)-\left(\frac{\omega_1-1}{z-1}\right)^{\alpha}\left(\frac{\omega_1+1}{z+1}\right)^{\beta}Q_0^{(\alpha,\beta)}(\omega_1)\right\}. \tag{4.17}$$

This identity was obtained earlier by Agrawal and Singh ([1, (2.10) and (2.11)]). It should be noted that these authors obtain for $Q_n^{(\alpha,\beta)}(z)$ an interesting generating function involving a F_3 which is not a special case of either (4.14) or (4.16).

Note that ω_2 maps the z interval $[-1,1]$ into itself. This fact allows us to average the values of expansion (4.17) above and below the cut.[5] The result is the analogous sum involving $\boldsymbol{Q}_n^{(\alpha,\beta)}(x)$.

$$\sum_{n=0}^{\infty}\lambda^n\boldsymbol{Q}_n^{(\alpha,\beta)}(x)=\frac{1}{(\lambda^2-2x\lambda+1)^{1/2}}$$
$$\times\left\{\left(\frac{1-\omega_2}{1-x}\right)^{\alpha}\left(\frac{1+\omega_2}{1+x}\right)^{\beta}\boldsymbol{Q}_0^{(\alpha,\beta)}(\omega_2)-\cos(\pi\alpha)\left(\frac{\omega_1-1}{1-x}\right)^{\alpha}\left(\frac{1+\omega_1}{1+x}\right)^{\beta}Q_0^{(\alpha,\beta)}(\omega_1)\right\}. \tag{4.18}$$

This series, which converges for $|\lambda|<1$, provides a very effective check on our computations. We used it with $\lambda=\frac{1}{2}$ to construct the entries in Table 2 which are discussed in Section 6.

[5] That is, above or below the cut, $\arg(\omega_2-1)=\arg(z-1)$, and principal values are taken as in Footnote 2. Each of the three functions $(\omega_1\pm1)$ and (ω_2+1) has the same value above and below the cut.

Table 2
The normalization relationship (4.18) for $\alpha = \beta = 6$, $\lambda = \frac{1}{2}$. The $Q_n^{(\alpha,\beta)}(\cos\theta)$ are computed from the recurrence relation (2.6) for $n = 0, 1, 2, \ldots, 200$

$\theta/°$	Numerical values of left and right-hand sides of (4.18)	Relative error	Absolute error
1	0.6385999372067(+21)	−0.218(−24)	−0.139(−03)
2	0.1563207978410(+18)	−0.502(−25)	−0.784(−08)
3	0.1210140203360(+16)	−0.683(−25)	−0.826(−10)
4	0.3857025831193(+14)	0.113(−24)	0.435(−11)
5	0.2671676255341(+13)	−0.938(−25)	−0.251(−12)
6	0.3025748174303(+12)	0.123(−24)	0.374(−13)
7	0.4813611867240(+11)	0.349(−25)	0.168(−14)
8	0.9825337257789(+10)	0.280(−25)	0.275(−15)
9	0.2427067703387(+10)	0.254(−25)	0.617(−16)
10	0.6971840826811(+09)	0.187(−24)	0.130(−15)
20	0.2240108209261(+06)	0.402(−25)	0.901(−20)
30	0.2836134830678(+04)	0.260(−24)	0.738(−21)
40	0.1845006217606(+03)	0.226(−24)	0.418(−22)
50	0.2724320269044(+02)	−0.628(−25)	−0.171(−23)
60	0.5325960309140(+01)	−0.193(−24)	−0.103(−23)
70	0.7010537003172(+00)	−0.450(−24)	−0.315(−24)
80	−0.4742844534822(+00)	0.354(−23)	−0.168(−23)
90	−0.8351489274557(+00)	0.161(−23)	−0.135(−23)
100	−0.1078183658097(+01)	−0.524(−24)	0.565(−24)
110	−0.1578054282012(+01)	0.174(−24)	−0.274(−24)
120	−0.3215734982933(+01)	0.962(−23)	−0.309(−22)
130	−0.1098043815182(+02)	−0.857(−24)	0.941(−23)
140	−0.7548202023354(+02)	−0.250(−23)	0.189(−21)
150	−0.1366348430114(+04)	0.137(−22)	−0.188(−19)
160	−0.1206296262916(+06)	0.192(−22)	−0.232(−17)
170	−0.3937690003811(+09)	0.114(−22)	−0.450(−14)
171	−0.1374448664824(+10)	0.732(−24)	−0.101(−14)
172	−0.5577155450693(+10)	0.160(−22)	−0.890(−13)
173	−0.2737950521967(+11)	−0.185(−23)	0.505(−13)
174	−0.1724054243917(+12)	0.107(−22)	−0.185(−11)
175	−0.1524555055732(+13)	0.271(−22)	−0.413(−10)
176	−0.2203601433714(+14)	0.234(−22)	−0.515(−09)
177	−0.6920214022645(+15)	−0.316(−22)	0.219(−07)
178	−0.8945149655381(+17)	−0.492(−23)	0.440(−06)
179	−0.3655707960795(+21)	0.226(−22)	−0.826(−02)

Note: The numbers in parentheses are the power of ten by which the entry must be multiplied.

5. Error studies

First we need some asymptotic results. The asymptotics of $Q_n^{(\alpha,\beta)}(z)$ off the cut are given in [8, vol. 1, p.77, (16)], or in [7, (2.14)]. We have

$$Q_n^{(\alpha,\beta)}(z) \sim \frac{1}{2}\left(\frac{\pi}{n}\right)^{1/2} \frac{[z+\sqrt{z^2-1}]^{N_{\alpha,\beta}}}{((z-1)/2)^{\alpha/2+1/4}((z+1)/2)^{\beta/2+1/4}}, \quad n \to \infty,$$

$$N_{\alpha,\beta} = n + \tfrac{1}{2}(\alpha+\beta+1), \quad z \notin [-1,1]. \tag{5.1}$$

From [12], we have on the cut,

$$Q_n^{(\alpha,\beta)}(x) \sim \frac{1}{2}\left(\frac{\pi}{n}\right)^{1/2} \frac{\cos(N_{\alpha,\beta}\theta + \Delta)}{[\sin(\theta/2)]^{\alpha+1/2}[\cos(\theta/2)]^{\beta+1/2}}, \quad n \to \infty,$$

$$\Delta = \tfrac{1}{2}(\alpha+1/2)\pi, \qquad x = \cos\theta, \qquad \varepsilon \leqslant \theta \leqslant \pi - \varepsilon, \tag{5.2}$$

for some $\varepsilon > 0$. This approximation also follows from results in [11, vol. 1, p.236, (7)].

For the Jacobi polynomials we have

$$P_n^{(\alpha,\beta)}(z) \sim \frac{1}{2}\left(\frac{1}{\pi n}\right)^{1/2} \frac{[z+\sqrt{z^2-1}]^{N_{\alpha,\beta}}}{((z-1)/2)^{\alpha/2+1/4}((z+1)/2)^{\beta/2+1/4}}, \quad n \to \infty, \tag{5.3}$$

off the cut, [18, p.196, (8.21.9)], and on the cut

$$P_n^{(\alpha,\beta)}(x) \sim \left(\frac{1}{\pi n}\right)^{1/2} \frac{\cos(N_{\alpha,\beta}\theta + \Omega)}{[\sin(\theta/2)]^{\alpha+1/2}[\cos(\theta/2)]^{\beta+1/2}}, \quad n \to \infty,$$

$$\Omega = -\tfrac{1}{2}(\alpha+1/2)\pi, \qquad x = \cos\theta, \qquad \varepsilon \leqslant \theta \leqslant \pi - \varepsilon, \tag{5.4}$$

for some $\varepsilon > 0$; see [18, p.196, (8.21.10)].

Chow et al. [3] have derived a beautiful inequality for $P_n^{(\alpha,\beta)}(x)$ which can be shown to hold for noninteger n, i.e., for Jacobi functions of the first kind. Thus, the inequality may be extended, via (2.4), to the function $Q_n^{(\alpha,\beta)}(x)$, since the functions on the right of (2.4) are Jacobi functions of the first kind of degrees n and $n+\alpha+\beta$, respectively. Unfortunately, the inequality holds only for $-\frac{1}{2} \leqslant \alpha, \beta \leqslant \frac{1}{2}$.[6] Remember, in our case α and/or β may be large. Lacking such an inequality, we will have to settle in our error studies for *asymptotic* inequality rather than inequality, i.e., we use the asymptotic approximations (5.2) and (5.4) to estimate the error, rather than the functions themselves. To make this idea less vague, we adopt the following convention. Let X denote the class of all complex sequences $\{\eta_n\}$ with the properties $\eta_n \neq 0$, $n = 0, 1, 2, \ldots,$ and $\eta_n = 1 + o(1)$ as $n \to \infty$.

[6] In a private communication, Roderick Wong has told us that he suspects the inequality fails if the conditions on α, β are violated.

It is easy to establish that for $\eta_n \in X$ and r fixed, γ real,

$$\sum_{k=r(>0)}^{n} \eta_k k^\gamma = \zeta_n \frac{n^{\gamma+1}}{\gamma+1}, \quad \gamma > -1, \tag{5.5}$$

for some $\zeta_n \in X$ and for $n > n_0$ for some n_0. Also if $\eta_n, \zeta_n \in X$,

$$\frac{\eta_n}{\zeta_n} = \xi_n, \qquad \eta_n \cdot \zeta_n = \chi_n, \tag{5.6}$$

for some $\xi_n, \chi_n \in X$.

The $Q_n^{(\alpha,\beta)}(x)$ are generated from the recurrence (2.6) by using it in the forward direction with the initial values $y_0(x) = Q_0^{(\alpha,\beta)}(x)$, $y_1(x) = Q_1^{(\alpha,\beta)}(x)$. What actually happens numerically is that we are computing with a recurrence of the form

$$y_{n+2}(x) + A_n(x) y_{n+1}(x) + B_n y_n(x) = \varepsilon_n, \quad n = 0, 1, 2, \dots, \tag{5.7}$$

where $\varepsilon_n = \varepsilon_n(x)$ denotes the error, arising from any source whatever, that occurs at the nth stage of the computation. We assume that the sequence ε_n is bounded, and denote its norm by

$$\|\varepsilon_n\| = \sup_{n \geqslant 0} |\varepsilon_n|. \tag{5.8}$$

The complete solution of (5.7) can be written

$$y_n(x) = C_1 y_n^{(1)}(x) + C_2 y_n^{(2)}(x) + y_n^{(p)}(x), \tag{5.9}$$

where $y_n^{(1)}(x)$, $y_n^{(2)}(x)$ are a set of linearly independent solutions of the related homogeneous equation (2.6), $y_n^{(p)}(x)$ is a particular solution of (5.7) and C_1 and C_2 are constants, see [20, Appendix A]. We can represent $y_n^{(p)}(x)$ as

$$y_n^{(p)}(x) = \sum_{k=0}^{n-1} \frac{y_{k+1}^{(1)}(x) y_n^{(2)}(x) - y_{k+1}^{(2)}(x) y_n^{(1)}(x)}{D_k(x) B_k} \varepsilon_k, \quad n = 0, 1, 2, \dots,$$

$$D_k(x) = y_k^{(1)}(x) y_{k+1}^{(2)}(x) - y_k^{(2)}(x) y_{k+1}^{(1)}(x). \tag{5.10}$$

(Empty sums are interpreted as 0.) The identical vanishing of $D_k(x)$ is a necessary and sufficient condition for the linear dependence of two solutions of the recurrence (see [20, Appendix A]) and (2.8) shows $y_n^{(1)}(x)$, $y_n^{(2)}(x)$ will be linearly independent if and only if $\alpha \neq$ half an odd integer. We assume this restriction on α holds in the remainder of this section. Also throughout we will assume $-1 + \varepsilon \leqslant x \leqslant 1 - \varepsilon$ for some $\varepsilon > 0$, i.e., x is kept away from the endpoints of $[-1, 1]$ by a positive amount.

We now choose

$$y_n^{(1)}(x) = P_n^{(\alpha,\beta)}(x), \qquad y_n^{(2)}(x) = Q_n^{(\alpha,\beta)}(x). \tag{5.11}$$

Eq. (2.8) gives

$$D_n(x) = -(1-x)^{-\alpha}(1+x)^{-\beta}\cos(\pi\alpha) 2^{\alpha+\beta-1}(2n+\alpha+\beta+2)\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+2)\Gamma(n+\alpha+\beta+2)}. \tag{5.12}$$

Note that $y_n^{(p)}(x) = 0$, for $n = 0, 1$ and $y_n^{(p)}(x) = \varepsilon_0$. This allows us to determine C_1, and C_2 in (5.9). We find $C_1 = 0$, $C_2 = 1$, so the solution of the recurrence actually computed is

$$y_n(x) = Q_n^{(\alpha,\beta)}(x) + y_n^{(p)}(x). \tag{5.13}$$

Using the relationship $\Gamma(n+a)/\Gamma(n+b) \sim n^{a-b}$ for $n \to \infty$, we find (5.12) simplifies to

$$D_n(x) \sim -\frac{1}{n}(1-x)^{-\alpha}(1+x)^{-\beta}\cos(\pi\alpha)2^{\alpha+\beta}, \quad n \to \infty. \tag{5.14}$$

Also from the definition of B_n in (2.6),

$$B_n \sim 1, \quad n \to \infty. \tag{5.15}$$

Straightforward but lengthy algebra using (5.2), (5.4), (5.10), (5.13)–(5.15), the properties (5.5) and (5.6) and the triangle inequality for the sum (5.10) results in the asymptotic inequality

$$|y_n(\cos\theta) - Q_n^{(\alpha,\beta)}(\cos\theta)| \leqslant \frac{4n\|\varepsilon_n\|}{3\sin\theta\,|\cos(\pi\alpha)|}\zeta_n, \quad 0 < \theta < \pi, \tag{5.16}$$

for some real positive $\zeta_n \in X$ and for $n > n_0$ for some n_0.

The above means that errors introduced randomly during the course of the computations grow at most algebraically with n, in fact, $O(n)$. Thus, forward computation for $Q_n^{(\alpha,\beta)}(x)$ is very stable. Problems occur, however, near the endpoints of the interval $\theta = 0, \pi$, where the error becomes very large. We shall go into more detail about this in the next section.

6. Some numerics

We used the following protocol for our computations:

1. α and β are held fixed throughout the calculation.
2. We set the argument to $\theta = 1°$.
3. All the $P_n^{(\alpha,\beta)}(\cos\theta)$ and all the $Q_n^{(\alpha,\beta)}(\cos\theta)$ were calculated for this argument, for the degree n ranging from 0 to some large upper limit. For the $P_n^{(\alpha,\beta)}(\cos\theta)$ this was done by first computing $P_0^{(\alpha,\beta)}(\cos\theta)$ and $P_1^{(\alpha,\beta)}(\cos\theta)$ in (4.2), and the remainder from the three-term recurrence relation (2.6). For the $Q_n^{(\alpha,\beta)}(\cos\theta)$ we did the same, using as starting values the expressions for $Q_0^{(\alpha,\beta)}(\cos\theta)$ and $Q_1^{(\alpha,\beta)}(\cos\theta)$ in Section 3. The remainder of the $Q_n^{(\alpha,\beta)}(\cos\theta)$ were obtained from the recurrence (2.6).
4. We made two checks on the computed values of the $P_n^{(\alpha,\beta)}(\cos\theta)$ and the $Q_n^{(\alpha,\beta)}(\cos\theta)$: we compared

   $$Q_{n-1}^{(\alpha,\beta)}(\cos\theta)P_n^{(\alpha,\beta)}(\cos\theta) - Q_n^{(\alpha,\beta)}(\cos\theta)P_{n-1}^{(\alpha,\beta)}(\cos\theta)$$

   with the right-hand side of the Casoratian identity (2.8), and we compared the generating function (4.18) computed for a large number of terms with the value of the sum given by the right-hand side.
5. If $\theta < 179°$, we incremented by 1° and returned to Step 3.

The computations were performed on the Hewlett-Packard Series 700 workstations using quadruple precision FORTRAN. This gives about 34 digits of precision.

Table 1 reports a test of the Casoratian identity (2.8) for $n = 200$, $\alpha = \beta = 6$ with $\theta = 1(1)9°$, then $\theta = 10(10)170°$ and finally $\theta = 171(1)179°$. A similar test of the generating function (4.18) is given in Table 2 using $n = 0(1)200$ and $\lambda = \frac{1}{2}$. In both tables the second column reports the common values to 13 significant figures of the right- and left-hand sides of (2.8) and (4.18). The third and fourth columns display the relative error = (rhs − lhs)/rhs and absolute error = rhs − lhs, respectively. Note the absolute error increases dramatically near the endpoints of the interval $\theta = 0, 180°$ although the relative error remains nearly constant.

The relative errors in Table 2 are many orders of magnitude larger than the corresponding ones in Table 1. This is because the computation of $Q_0^{(\alpha,\beta)}(\omega_1)$ in (4.18) involves the subtraction of two nearly equal quantities. For example, consider the case $x = 0$ (i.e., $\theta = 90°$) in Table 2. With the help of *Mathematica* [22], we find for the terms on the right-hand side of (4.18), $\omega_2 = 2 - \sqrt{5}$, $\omega_1 = 2 + \sqrt{5}$, $(\lambda^2 + 1)^{-1/2} = 2/\sqrt{5}$, $(1 - \omega_2)^6 = 576 - 256\sqrt{5}$, $(1 + \omega_2)^6 = 10304 - 4608\sqrt{5}$, $(\omega_1 - 1)^6 = 576 + 256\sqrt{5}$, $(\omega_1 + 1)^6 = 10304 + 4608\sqrt{5}$, and

$$Q_0^{(6,6)}(\omega_2) = \frac{-379}{630} - \frac{895\sqrt{5}}{5544} + \frac{1}{2}\ln\left[\tfrac{1}{2}(\sqrt{5} - 1)\right] \approx -1.203,$$

$$Q_0^{(6,6)}(\omega_1) = \frac{-379}{630} + \frac{895\sqrt{5}}{5544} + \frac{1}{2}\ln\left[\tfrac{1}{2}(\sqrt{5} + 1)\right] \approx 3.414 \times 10^{-9}.$$

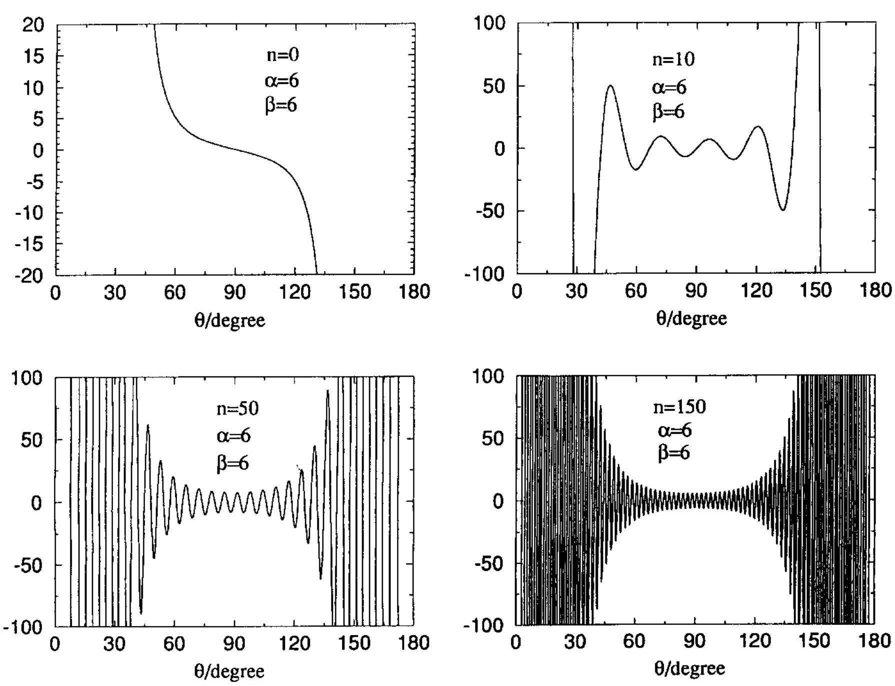

Fig 1. Plot of the Jacobi function $Q_n^{(\alpha,\beta)}(\cos\theta)$ for four values of n and $\alpha = 6$, $\beta = 6$.

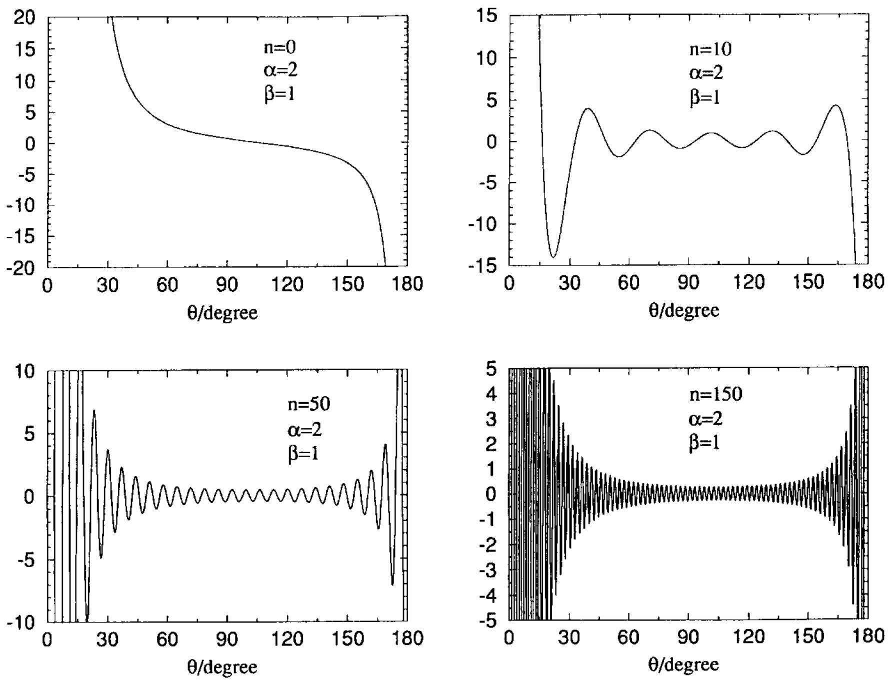

Fig 2. Plot of the Jacobi function $Q_n^{(\alpha,\beta)}(\cos\theta)$ for four values of n and $\alpha = 2$, $\beta = 1$.

As a further check, we used the arbitrary precision capabilities of *Mathematica* to evaluate (4.18) for the case just discussed. For a cutoff value of $n = 200$, the absolute error is -1.272×10^{-60} which decreases to -8.477×10^{-91} for $n = 300$.

Fig. 1 plots $Q_n^{(\alpha,\beta)}(\cos\theta)$ vs. θ for $\alpha = \beta = 6$ and $n = 0, 10, 50, 150$ while Fig. 2 displays graphs for the same values of n but with $\alpha = 2$, $\beta = 1$. These figures clearly show that $Q_n^{(\alpha,\beta)}(\cos\theta)$ becomes violently oscillatory and unbounded near the endpoints of the interval.

7. Concluding remarks

After this paper was delivered at the CAM conference of 1996, Kai Diethelm of Universität Hildesheim made several interesting observations. First, he noticed that the error in Table 1 is not symmetric, though the function being computed and the Casoratian relationship are. This, no doubt, is due to the asymmetry of the small randomly induced errors introduced at each stage of the machine computation. His second comment was that a check on $Q_n^{(\alpha,\beta)}(\cos\theta)$ for the largest value of n for which the function is computed may be obtained by using the principal value integral representation for the function and applying to this integral the quadrature methods he had discussed in his own conference presentation. We thought this an excellent suggestion, and refer the reader to that conference contribution, "Error bound for Cauchy principal value quadratures using L_p norms and total variation," and to the references therein.

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